1-Methoxy-2-propyl acetate 108-65-6 | DTXSID1026796

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 1.01 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.77e-01

Confidence level: 7.49e-01

Nearest Neighbors from the Training Set

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1-Methoxy-2-propyl acetate

Measured: 1.50 Predicted: 1.01

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2-Ethoxyethyl acetate

Measured: 1.87 Predicted: 9.80e-01

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Methyl 3-ethoxypropanoate

Measured: 8.47e-01 Predicted: 1.24

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propyl 3-methoxypropanoate

Measured: 2.19e-01 Predicted: 2.08e-01

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Ethyl 3-ethoxypropionate Measured: 3.80e-01 Predicted: 2.06e-01